tert-Butylhydroquinone

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 3.44

Global applicability domain: Inside

Local applicability domain index: 4.97e-01

Confidence level: 7.86e-01

Nearest Neighbors from the Training Set

Image not found
2-tert-Butylphenol
Measured: 3.31
Predicted: 3.34

Image not found
3-tert-Butylphenol
Measured: 3.30
Predicted: 3.44

Image not found
4-tert-Butylphenol
Measured: 3.31
Predicted: 3.44

Image not found
4-tert-Butylbenzoic acid
Measured: 3.85
Predicted: 3.43

Image not found
4-Hexylresorcinol
Measured: 3.45
Predicted: 3.66